Rosiaite ($PbSb_2O_6$) Structure: A6BC2_hP9_162_k_a_d-001

This structure previously used the label(s) `A6BC2_hP9_162_k_a_d`. Calls to these addresses will be redirected here.

Cite this page as:

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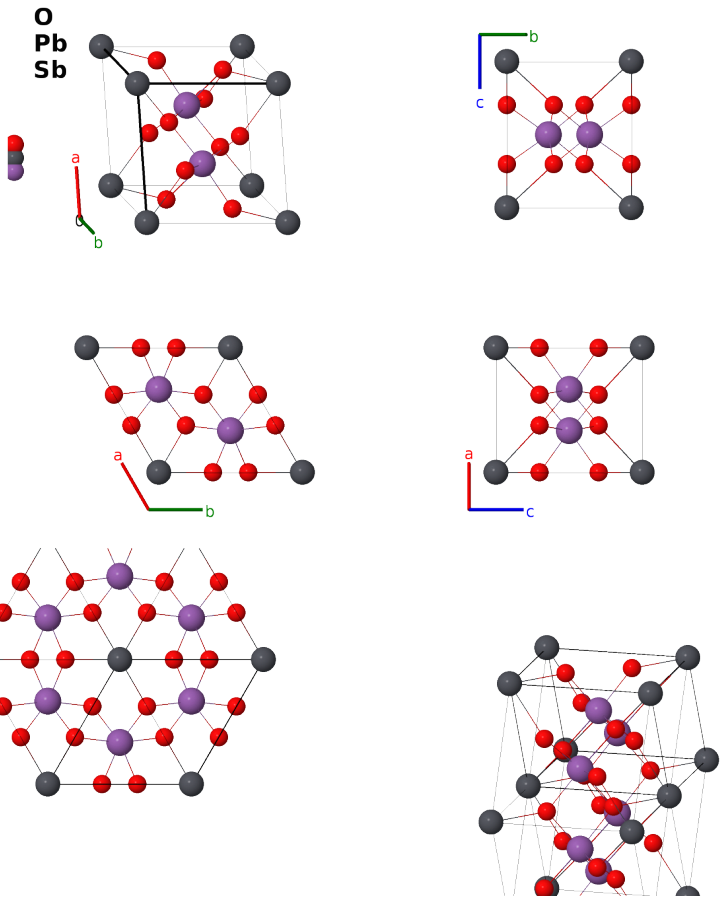
https://aflow.org/prototype-encyclopedia/80KE

https://aflow.org/prototype-encyclopedia/A6BC2_hP9_162_k_a_d-001



Prototype	O_6PbSb_2
AFLOW prototype label	A6BC2_hP9_162_k_a_d-001
Mineral name	rosiaite
ICSD	81387
CCDC	1641529
Pearson symbol	hP9
Space group number	162

Space group symbol $P\bar{3}1m$

AFLOW prototype command `aflow --proto=A6BC2_hP9_162_k_a_d-001 --params=`$a, c/a, x_3, z_3$

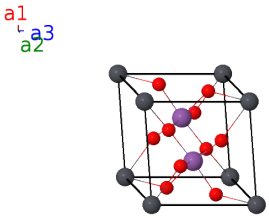
Other compounds with this structure

$BaSb_2O_6$, $CaAs_2O_6$, $CaOs_2O_6$, $CaSb_2O_6$, $CdAs_2O_6$, $CdSb_2O_6$, $CoAs_2O_6$, $HfLi_2F_6$, $HgAs_2O_6$, $MnAs_2O_6$, $MnSb_2O_6$, $MoLi_2F_6$, $NbLi_2F_6$, $NiAs_2O_6$, $PbAs_2O_6$, $PbLi_2F_6$, $PbSb_2O_6$, $PdAs_2O_6$, $SrAs_2O_6$, $SrRu_2O_6$, $SrSb_2O_6$, UCr_2O_6, UV_2O_6, $ZrLi_2F_6$, $MnSeTeO_6$, $MnSnTeO_6$, $PbTeGeO_6$, $SrIr_2O_6$

- This is the ternary form of the $L'3_2$ (β-V_2N) structure.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Pb I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	Sb I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	Sb I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6k)	O I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - cz_3\,\hat{\mathbf{z}}$	(6k)	O I

References

[1] R. Basso, G. Lucchetti, L. Zefiro, and A. Palenzona, *Rosiaite, $PbSb_2O_6$, a new mineral from the Cetine mine, Siena, Italy*, Eur. J. of Mineral. **8**, 487–492 (1996).

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